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NON-LINEAR EFFECTS IN INTERACTIONS OF FAST IONS WITH GRAPHENE

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Abstract. We study the interactions of fast ions with graphene, describing the high-frequency plasmon excitations of the electron gas by a two-dimensional, two-fluid hydrodynamic model. The Barkas effect on the stopping force and the analogous correction to the image force are evaluated within the second-order perturbation approach to the hydrodynamic equations.

1. INTRODUCTION

Graphene is a single sheet of carbon atoms tightly packed into a two-dimensional (2D) honeycomb lattice (Novoselov et al. 2004). Besides being the fundamental building block of highly oriented pyrolytic graphite (HOPG), carbon nanotubes and fullerene molecules, graphene is currently attracting a great deal of interest on its own right owing to its fascinating physical properties, most notably as a potential basis for the future nano-electronic devices (Geim and Novoselov 2007, Katsnelson 2007, Katsnelson et al. 2006, Novoselov et al. 2006, Niyogi et al. 2006).

In the present paper, we adopt the hydrodynamic model of a 2D electron gas (Hetter 1973) to evaluate the stopping force and the image force which, in the regime of high projectile speeds and large distances from graphene, respectively, describe the dissipation of the projectile's kinetic energy into plasmon excitations in graphene, and the conservative force attracting the projectile towards graphene.

2. BASIC THEORY

We use a three-dimensional Cartesian coordinate system with $\overrightarrow{r} = (\overrightarrow{R}, z)$, where $\overrightarrow{R} = (x, y)$ is position in the graphene plane and z distance from it. Furthermore, we consider the ion to be a point charge Q, moving parallel to the graphene in the upper half-space defined by $z > 0$, with a constant velocity v, at distance z_0. Next, we describe the σ and π electrons in graphene as two fluids occupying the xy plane and having the equilibrium number densities per unit area $n_\sigma^0 \approx 0.321$ and $n_\pi^0 \approx 0.107$, respectively. The perturbations of their densities $n_j^{(1)}(\overrightarrow{R}, t)$ and their velocity fields $\overrightarrow{u}_j^{(1)}(\overrightarrow{R}, t)$, with $j = \sigma, \pi$, satisfy the linearized continuity equation and the linearized momentum-balance equation (Radović et al. 2007). The second-order equations are:

$$\frac{\partial n_j^{(2)}(\overrightarrow{R},\, t)}{\partial t} + n_j^0 \nabla_{||} \cdot \overrightarrow{u}_j^{(2)}(\overrightarrow{R},\, t) = -\nabla_{||} \cdot [n_j^{(1)}(\overrightarrow{R},\, t)\overrightarrow{u}_j^{(1)}(\overrightarrow{R},\, t)] \tag{1}$$

$$\begin{aligned}&\frac{\partial \overrightarrow{u}_j^{(2)}(\overrightarrow{R},t)}{\partial t} = \nabla_{||}\Phi_{tot}^{(2)}(\overrightarrow{R},\, z,\, t)\,|_{z=0} - \frac{\alpha_j}{n_j^0}\nabla_{||}n_j^{(2)}(\overrightarrow{R},\, t) - \gamma_j\overrightarrow{u}_j^{(2)}(\overrightarrow{R},\, t)\\ &-[\overrightarrow{u}_j^{(1)}(\overrightarrow{R},\, t)\cdot\nabla_{||}]\overrightarrow{u}_j^{(1)}(\overrightarrow{R},\, t)\end{aligned} \tag{2}$$

It can be noticed that, in Eqs. (1) and (2), $\nabla_{||} = \partial \big/ \partial\overrightarrow{R}$ differentiates in directions parallel to the xy plane. The first term on the right-hand side of Eq. (2) is the tangential force on an electron due to the total electric field at $z = 0$, where $\Phi_{tot}^{(2)}(\overrightarrow{R},\, z,\, t) \equiv \Phi_{ind}^{(2)}(\overrightarrow{R},\, z,\, t)$ because we assume that ρ_{ext} is a weak, first-order perturbation of the 2D electron gas. The second term describes the internal interactions in the electron fluids based on the Thomas-Fermi model (van Zyl and Zaremba 1999, Parr and Yang 1989), giving $\alpha_j = \pi n_j^0$. The third term in Eq. (2) represents phenomenologically introduced friction in the electron gas with the friction constant γ_j which we take to be infinitesimally small.

These equations are solved by performing the Fourier transformation in the xy plane and in time ($\overrightarrow{R} \to \overrightarrow{k}$ and $t \to \omega$). After some algebra, one can obtain the Fourier transform of the second-order induced density $n_2(\overrightarrow{k},\, \omega) = n_\sigma^{(2)}(\overrightarrow{k},\, \omega) + n_\pi^{(2)}(\overrightarrow{k},\, \omega)$. By performing the inverse Fourier transformation in the xy plane and in time ($\overrightarrow{k} \to \overrightarrow{R}$ and $\omega \to t$), we obtain the second-order expression for the induced potential as:

$$\begin{aligned}&\Phi_{ind}^{(2)}(\overrightarrow{R},\, z,\, t) =\\ &\sum_{j=\sigma,\pi}\Bigg[\frac{Q^2}{4\pi(n_j^0)^2}\int\frac{(\overrightarrow{k}-\overrightarrow{k}')\cdot\overrightarrow{v}\left[k^2(\overrightarrow{k}'\cdot\overrightarrow{v})\overrightarrow{k}'\cdot(\overrightarrow{k}-\overrightarrow{k}')+2(\overrightarrow{k}\cdot\overrightarrow{v}+i\gamma_j)k'^2\overrightarrow{k}\cdot(\overrightarrow{k}-\overrightarrow{k}')\right]}{k^3k'^3|\overrightarrow{k}-\overrightarrow{k}'|^3D(k,\,\overrightarrow{k}\cdot\overrightarrow{v})D(k',\,\overrightarrow{k}'\cdot\overrightarrow{v})D(|\overrightarrow{k}-\overrightarrow{k}'|,(\overrightarrow{k}-\overrightarrow{k}')\cdot\overrightarrow{v})}\\ &\times\chi_j(k,\,\overrightarrow{k}\cdot\overrightarrow{v})\chi_j(k',\,\overrightarrow{k}'\cdot\overrightarrow{v})e^{-(k'+|\overrightarrow{k}-\overrightarrow{k}'|)z_0}e^{-kz}e^{i\overrightarrow{k}\cdot(\overrightarrow{R}-\overrightarrow{v}t)}d^2\overrightarrow{k}\,d^2\overrightarrow{k}'\Bigg]\end{aligned} \tag{3}$$

where $D(k,\, \omega) = 1 + \frac{2\pi}{k}\chi(k,\, \omega)$. The polarization function of graphene is given by $\chi(k,\, \omega) = \sum_{j=\sigma,\pi}\chi_j(k,\, \omega)$ with $\chi_j(k,\, \omega) = \frac{n_j^0 k^2}{\alpha_j k^2 - \omega(\omega + i\gamma_j)}$.

3. RESULTS FOR STOPPING AND IMAGE FORCES

The stopping force is defined by $F_s = -Q\,\hat{\overrightarrow{v}}\cdot\nabla_{||}\Phi_{ind}(\overrightarrow{R},\, z,\, t)\Big|_{\overrightarrow{R}=\overrightarrow{v}t,\, z=z_0}$, with the derivative $\nabla_{||}\Phi_{ind}(\overrightarrow{R},\, z,\, t)$ taken at the ion position ($\overrightarrow{R} = \overrightarrow{v}t$, $z = z_0$) and $\hat{\overrightarrow{v}}$ being the unit vector in the direction of ion's motion. The image force is defined by $F_{im} = -Q\frac{\partial}{\partial z}\Phi_{ind}(\overrightarrow{R},\, z,\, t)\Big|_{\overrightarrow{R}=\overrightarrow{v}t,\, z=z_0}$.

The second-order expressions for the stopping and image forces are, respectively:

$$F_s^{(2)} = -\sum_{j=\sigma,\pi}\left[\frac{iQ^3}{2\pi v(n_j^0)^2}\int_0^\infty \frac{e^{-kz_0}}{k^2}dk\int_0^\infty \frac{e^{-k'z_0}}{k'^2}dk'\int_{-kv}^{kv}\frac{\omega\chi_j(k,\omega)d\omega}{D(k,\omega)\sqrt{k^2v^2-\omega^2}}\right.$$
$$\left.\times\int_{-k'v}^{k'v}\frac{\chi_j(k',\omega')\left[\frac{A_j\chi_j(B,\omega-\omega')}{B^3D(B,\omega-\omega')}e^{-Bz_0}+\frac{A'_j\chi_j(B',\omega-\omega')}{B'^3D(B',\omega-\omega')}e^{-B'z_0}\right]}{D(k',\omega')\sqrt{k'^2v^2-\omega'^2}}d\omega'\right] \quad (4)$$

$$F_{im}^{(2)} = \sum_{j=\sigma,\pi}\left[\frac{Q^3}{2\pi(n_j^0)^2}\int_0^\infty \frac{e^{-kz_0}}{k}dk\int_0^\infty \frac{e^{-k'z_0}}{k'^2}dk'\int_{-kv}^{kv}\frac{\chi_j(k,\omega)d\omega}{D(k,\omega)\sqrt{k^2v^2-\omega^2}}\right.$$
$$\left.\times\int_{-k'v}^{k'v}\frac{\chi_j(k',\omega')\left[\frac{A_j\chi_j(B,\omega-\omega')}{B^3D(B,\omega-\omega')}e^{-Bz_0}+\frac{A'_j\chi_j(B',\omega-\omega')}{B'^3D(B',\omega-\omega')}e^{-B'z_0}\right]}{D(k',\omega')\sqrt{k'^2v^2-\omega'^2}}d\omega'\right] \quad (5)$$

where $A_j = (\omega - \omega')\left[k^2\omega'\left(\frac{C}{v^2} - k'^2\right) + 2(\omega + i\gamma_j)k'^2\left(k^2 - \frac{C}{v^2}\right)\right]$ and $B = \sqrt{k^2 + k'^2 - 2C/v^2}$ with $C = \omega\omega' + \sqrt{k^2v^2 - \omega^2}\sqrt{k'^2v^2 - \omega'^2}$, while in the expressions for A'_j and B' one has to replace C by $C' = \omega\omega' - \sqrt{k^2v^2 - \omega^2}\sqrt{k'^2v^2 - \omega'^2}$.

Note that the second-order expressions for the stopping and image forces are each proportional to Q^3 (so-called Barkas effect (Barkas et al. 1963)) and are therefore sensitive to the sign of the external charge, in contrast to the first-order expressions for these forces (Radović et al. 2007).

4. CONCLUSION

We have used a simple 2D, two-fluid model to describe the high-frequency collective electron excitations in graphene. The Barkas correction to the stopping force and the analogous corrections to the induced potential and the image force on charged particles moving parallel to graphene have been obtained by means of the second-order perturbation of the hydrodynamic equations. In future work, we shall evaluate numerically expressions (4) and (5) for those forces to establish the range of relevant parameters validating the applicability of the linearized hydrodynamic model.

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